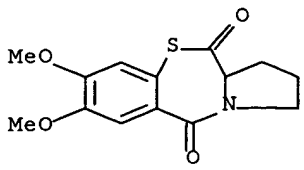
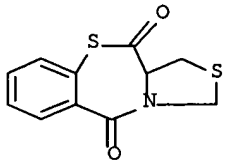
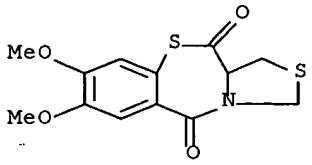
L4 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 2002:813788 CAPLUS
DN 138:265140
TI 3D-QSAR and molecular modeling of HIV-1 integrase inhibitors
AU Makhija, Mahindra T.; Kulkarni, Vithal M.
CS Pharmaceutical Division, Department of Chemical Technology, University of Mumbai, Mumbai, 400 019, India
SO Journal of Computer-Aided Molecular Design (2002), 16(3), 181-200
CODEN: JCADEQ; ISSN: 0920-654X
PB Kluwer Academic Publishers
DT Journal
LA English
AB Three-dimensional quant. structure-activity relationship (3D QSAR) methods were applied on a series of inhibitors of HIV-1 integrase with respect to their inhibition of 3'-processing and 3'-end joining steps in vitro. The training set consisted of 27 compds. belonging to the class of thiazolothiazepines. The predictive ability of each model was evaluated using test set I consisting of four thiazolothiazepines and test set II comprised of seven compds. belonging to an entirely different structural class of coumarins. Maximum Common Substructure (MCS) based method was used to align the mols. and this was compared with other known methods of alignment. Two methods of 3D QSAR: comparative mol. field anal. (CoMFA) and comparative mol. similarity indexes anal. (CoMSIA) were analyzed in terms of their predictive abilities. CoMSIA produced significantly better results for all correlations. The results indicate a strong correlation between the inhibitory activity of these compds. and the steric and electrostatic fields around them. CoMSIA models with considerable internal as well as external predictive ability were obtained. A poor correlation obtained with hydrophobic field indicates that the binding of thiazolothiazepines to HIV-1 integrase is mainly enthalpic in nature. Further the most active compd. of the series was docked into the active site using the crystal structure of integrase. The binding site was formed by the amino acid residues 64-67, 116, 148, 151-152, 155-156, and 159. The comparison of coeff. contour maps with the steric and electrostatic properties of the receptor shows high level of compatibility.
IT **125262-81-9 151324-42-4 151324-43-5**
151324-45-7 151324-46-8 151324-47-9
244610-00-2 244610-01-3 244610-02-4
244610-03-5 244610-04-6 244610-05-7
244610-06-8 244610-07-9 244610-08-0
244610-09-1 244610-10-4 244610-13-7
244610-14-8 244610-15-9 244610-16-0
244610-17-1 244626-16-2 244626-17-3
244626-18-4 306274-75-9 306274-76-0
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (3D-QSAR and mol. modeling of HIV-1 integrase inhibitors)
RN 125262-81-9 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



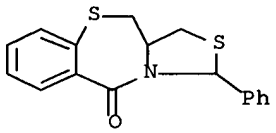
RN 151324-42-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-(9CI) (CA INDEX NAME)



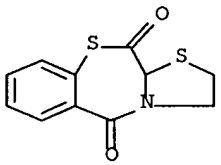
RN 151324-43-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



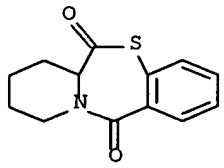
RN 151324-45-7 CAPLUS
CN 1H,3H,5H-Thiazolo[4,3-c][1,4]benzothiazepin-5-one, 11,11a-dihydro-3-phenyl-(9CI) (CA INDEX NAME)



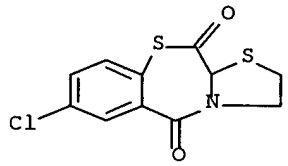
RN 151324-46-8 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-(9CI) (CA INDEX NAME)



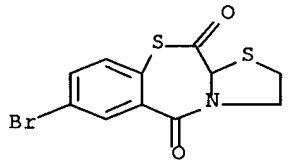
RN 151324-47-9 CAPLUS
CN 12H-Pyrido[2,1-c][1,4]benzothiazepine-6,12(6aH)-dione, 7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)



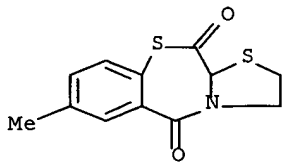
RN 244610-00-2 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-chloro-2,3-dihydro- (9CI) (CA INDEX NAME)



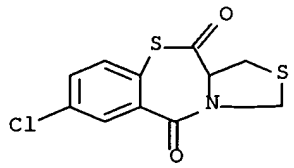
RN 244610-01-3 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-bromo-2,3-dihydro- (9CI) (CA INDEX NAME)



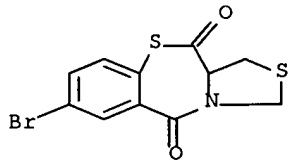
RN 244610-02-4 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl- (9CI) (CA INDEX NAME)



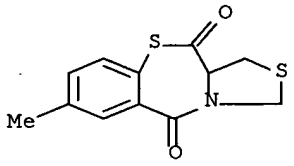
RN 244610-03-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-chloro-1,11a-dihydro- (9CI) (CA INDEX NAME)



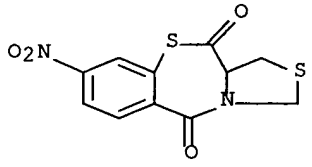
RN 244610-04-6 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-bromo-1,11a-dihydro- (9CI) (CA INDEX NAME)



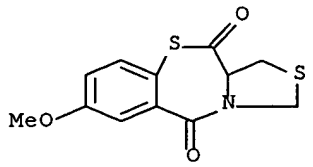
RN 244610-05-7 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methyl- (9CI) (CA INDEX NAME)



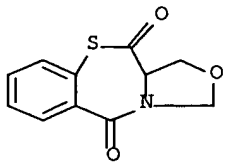
RN 244610-06-8 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-8-nitro- (9CI) (CA INDEX NAME)



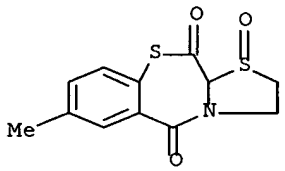
RN 244610-07-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



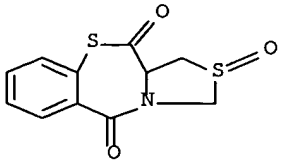
RN 244610-08-0 CAPLUS
CN 3H,5H,11H-Oxazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro- (9CI) (CA INDEX NAME)



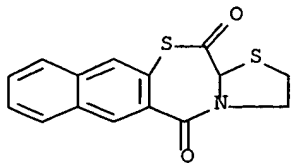
RN 244610-09-1 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl-, 1-oxide (9CI) (CA INDEX NAME)



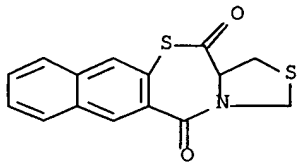
RN 244610-10-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-
,
2-oxide (9CI) (CA INDEX NAME)



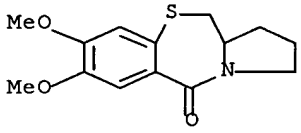
RN 244610-13-7 CAPLUS
CN 5H-Naphtho[2,3-f]thiazolo[2,3-c][1,4]thiazepine-5,13(13aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)



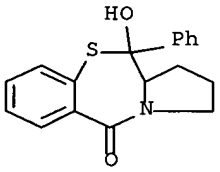
RN 244610-14-8 CAPLUS
CN 3H,5H,13H-Naphtho[2,3-f]thiazolo[4,3-c][1,4]thiazepine-5,13-dione, 1,13a-dihydro- (9CI) (CA INDEX NAME)



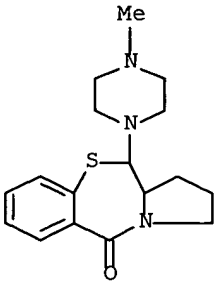
RN 244610-15-9 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



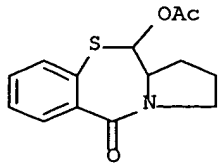
RN 244610-16-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy-11-phenyl- (9CI) (CA INDEX NAME)



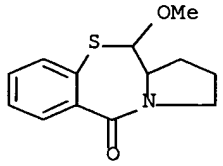
RN 244610-17-1 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



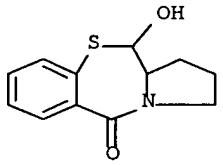
RN 244626-16-2 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-(acetyloxy)-2,3,11,11a-tetrahydro- (9CI) (CA INDEX NAME)



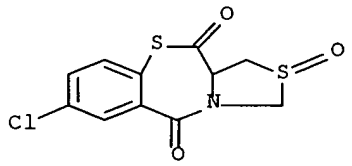
RN 244626-17-3 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-methoxy- (9CI) (CA INDEX NAME)



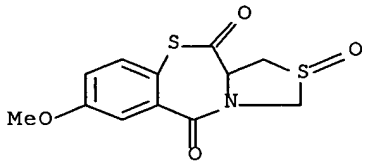
RN 244626-18-4 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy- (9CI) (CA INDEX NAME)



RN 306274-75-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-chloro-1,11a-dihydro-, 2-oxide (9CI) (CA INDEX NAME)

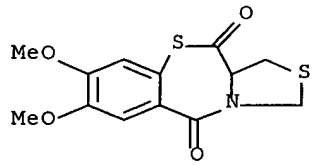


RN 306274-76-0 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy-, 2-oxide (9CI) (CA INDEX NAME)

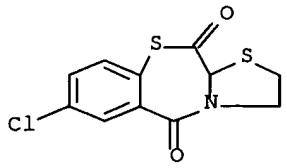


RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

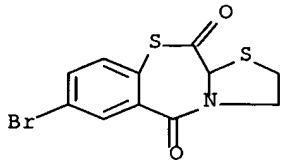
L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 2002:324031 CAPLUS
DN 137:272786
TI Molecular electrostatic potentials as input for the alignment of HIV-1 integrase inhibitors in 3d QSAR
AU Makhija, Mahindra T.; Kulkarni, Vithal M.
CS Pharmaceutical Division, Department of Chemical Technology, University of Mumbai, Mumbai, 400 019, India
SO Journal of Computer-Aided Molecular Design (2002), Volume Date 2001, 15(11), 961-978
CODEN: JCADEQ; ISSN: 0920-654X
PB Kluwer Academic Publishers
DT Journal
LA English
AB Comparative mol. similarity indexes anal. (CoMSIA), a three-dimensional quant. structure activity relation (3D QSAR) paradigm, was used to examine the correlations between the calcd. physicochem. properties and the in vitro activities (3'-processing and 3'-strand transfer inhibition) of a series of human immunodeficiency virus type 1 (HIV-1) integrase inhibitors. The training set consisted of 34 mols. from five structurally diverse classes: salicylpyrazolinones, dioxepinones, coumarins, quinones, and benzoic hydrazides. The data set was aligned using extrema of mol. electrostatic potentials (MEPs). The predictive ability of the resultant model was evaluated using a test set comprised of 7 mols. belonging to a different structural class of thiazepinediones. A CoMSIA model using an MEP-based alignment showed considerable internal as well external predictive ability (r2cv = 0.821, r2pred. = 0.608 for 3'-processing; and r2cv = 0.759, r2pred. = 0.660 for 3'-strand transfer).
IT **151324-43-5 244610-00-2 244610-01-3 244610-02-4 244610-07-9 244610-13-7 244610-14-8**
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(mol. electrostatic potentials as input for alignment of HIV-1 integrase inhibitors in 3d QSAR)
RN 151324-43-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



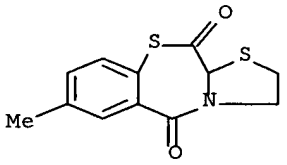
RN 244610-00-2 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-chloro-2,3-dihydro- (9CI) (CA INDEX NAME)



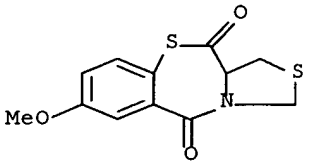
RN 244610-01-3 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-bromo-2,3-dihydro- (9CI) (CA INDEX NAME)



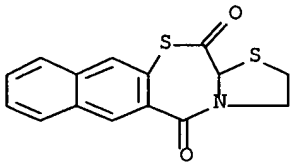
RN 244610-02-4 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl- (9CI) (CA INDEX NAME)



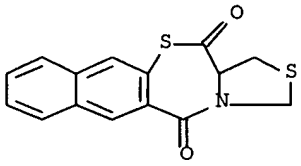
RN 244610-07-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



RN 244610-13-7 CAPLUS
CN 5H-Naphtho[2,3-f]thiazolo[2,3-c][1,4]thiazepine-5,13(13aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)

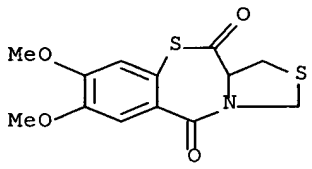


RN 244610-14-8 CAPLUS
CN 3H,5H,13H-Naphtho[2,3-f]thiazolo[4,3-c][1,4]thiazepine-5,13-dione, 1,13a-dihydro- (9CI) (CA INDEX NAME)

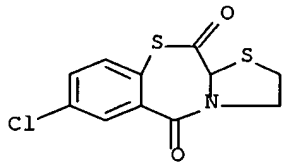


RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

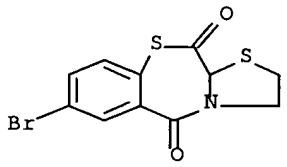
L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 2002:170729 CAPLUS
DN 137:210398
TI QSAR of HIV-1 integrase inhibitors by genetic function approximation method
AU Makhija, Mahindra T.; Kulkarni, Vithal M.
CS Department of Chemical Technology, Pharmaceutical Division, University of Mumbai, Matunga, Mumbai, 400 019, India
SO Bioorganic & Medicinal Chemistry (2002), 10(5), 1483-1497
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
AB Quant. structure-activity relation (QSAR) paradigm, using genetic function approxn. (GFA) technique was used to examine the correlations between the calcd. physicochem. descriptors and the in vitro activities (3'-processing and 3'-strand transfer inhibition) of a series of human immunodeficiency virus type 1 (HIV-1) integrase inhibitors. Depending on the chem. structure, all mols. were divided into two classes-catechols and noncatechols. Eighty-one mols. were used in the present study and they were divided into training set and test set. The training set in each class consisted of 35 mols. and QSAR models were generated sep. for both catechols and noncatechols. Equations were evaluated using internal as well as external test set predictions. Models generated for catechols show that electronic, shape related, and thermodn. parameters are important whereas for noncatechols, spatial, structural, and thermodn. properties play an important role for the activity.
IT **151324-43-5 244610-00-2 244610-01-3 244610-02-4 244610-07-9 244610-13-7 244610-14-8**
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(QSAR of HIV-1 integrase inhibitors by genetic function approxn. method)
RN 151324-43-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



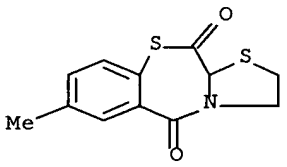
RN 244610-00-2 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-chloro-2,3-dihydro- (9CI) (CA INDEX NAME)



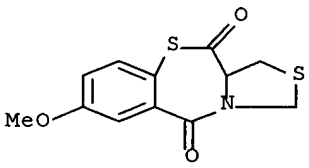
RN 244610-01-3 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-bromo-2,3-dihydro- (9CI) (CA INDEX NAME)



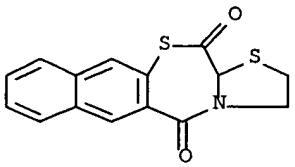
RN 244610-02-4 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl- (9CI) (CA INDEX NAME)



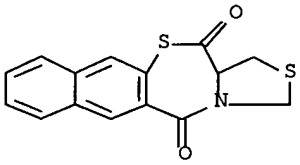
RN 244610-07-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



RN 244610-13-7 CAPLUS
CN 5H-Naphtho[2,3-f]thiazolo[2,3-c][1,4]thiazepine-5,13(13aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)

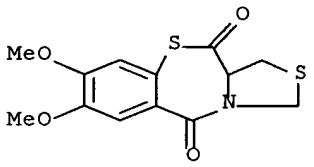


RN 244610-14-8 CAPLUS
CN 3H,5H,13H-Naphtho[2,3-f]thiazolo[4,3-c][1,4]thiazepine-5,13-dione, 1,13a-dihydro- (9CI) (CA INDEX NAME)

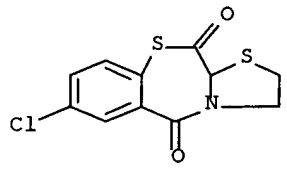


RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

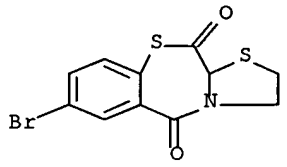
L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 2001:729988 CAPLUS
DN 136:195
TI Eigen Value Analysis of HIV-1 Integrase Inhibitors
AU Makhija, Mahindra T.; Kulkarni, Vithal M.
CS Pharmaceutical Division Department of Chemical Technology, University of Mumbai, Matunga, Mumbai, 400 019, India
SO Journal of Chemical Information and Computer Sciences (2001), 41(6), 1569-1577
CODEN: JCISD8; ISSN: 0095-2338
PB American Chemical Society
DT Journal
LA English
AB A three-dimensional quant. structure activity relation using the eigen value anal. (EVA) paradigm applied to 41 HIV-1 integrase inhibitors that inhibit integrase mediated cleavage (3'-processing step) and integration (3'-strand transfer step) in vitro was performed. The training set consisted of 35 mols. from five structurally diverse classes: salicylhydrazines, lichen acids, coumarins, quinones, and thiazolothiazepines. Models derived using semiempirical (MOPAC AM1 and PM3) calcd. normal-mode frequencies were compared. The predictive ability of each resultant model was evaluated using a test set comprised of six mols. belonging to a different structural class: hydrazides. Models derived using AM1 method showed considerable internal as well as external predictivity (r2cv = 0.806, r2pred = 0.761 for 3'-processing and r2cv = 0.677, r2pred = 0.591 for 3'-strand transfer).
IT **151324-43-5 244610-00-2 244610-01-3 244610-02-4 244610-07-9 244610-13-7 244610-14-8**
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Eigen value QSAR anal. of HIV-1 integrase inhibitors)
RN 151324-43-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



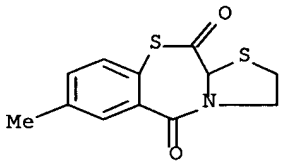
RN 244610-00-2 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-chloro-2,3-dihydro- (9CI) (CA INDEX NAME)



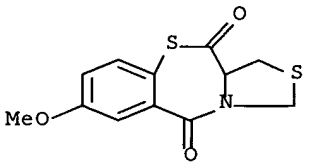
RN 244610-01-3 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-bromo-2,3-dihydro- (9CI) (CA INDEX NAME)



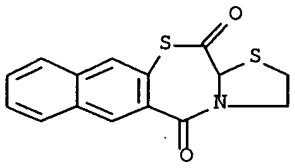
RN 244610-02-4 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl- (9CI) (CA INDEX NAME)



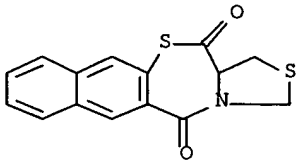
RN 244610-07-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



RN 244610-13-7 CAPLUS
CN 5H-Naphtho[2,3-f]thiazolo[2,3-c][1,4]thiazepine-5,13(13aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)



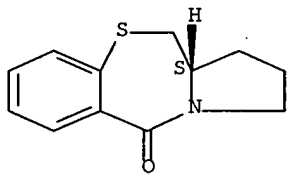
RN 244610-14-8 CAPLUS
CN 3H,5H,13H-Naphtho[2,3-f]thiazolo[4,3-c][1,4]thiazepine-5,13-dione, 1,13a-dihydro- (9CI) (CA INDEX NAME)



RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 2001:178041 CAPLUS
DN 135:5231
TI Base-promoted aminoethylation of thiols with 2-oxazolidinones: a simple synthesis of 2-aminoethyl sulfides
AU Ishibashi, H.; Uegaki, M.; Sakai, M.; Takeda, Y.
CS Faculty of Pharmaceutical Sciences, Kanazawa University, Takara-machi, Kanazawa, 920-0934, Japan
SO Tetrahedron (2001), 57(11), 2115-2120
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 135:5231
AB A simple synthesis of 2-aminoethyl sulfides using a base-promoted reaction of 2-oxazolidinones with thiols is described. An application of this method to the synthesis of chiral 2-aminoethyl sulfides and sulfur-contg. heterocyclic compds. is also presented.
IT **121451-33-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of of 2-aminoethyl sulfides by base-promoted aminoethylation of thiols with 2-oxazolidinones)
RN 121451-33-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-, (11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



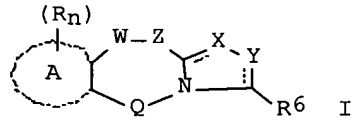
RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

App'S

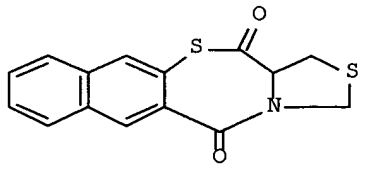
L4 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 2000:814491 CAPLUS
DN 133:350256
TI Preparation of benzothiazepines as inhibitors of HIV-1 integrase
IN Neamati, Nouri; Pommier, Yves; Garofalo, Antonio; Nacci, Vito
PA United States Dept. of Health and Human Services, USA
SO PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000068235	A1	20001116	WO 2000-US12847	20000510
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1187837	A1	20020320	EP 2000-932279	20000510
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	US 1999-133726P	P	19990512		
	WO 2000-US12847	W	20000510		

OS MARPAT 133:350256
GI



I



II

AB Title compds. [I; A = thiazole, benzene, naphthalene, pyridine, pyrimidine, pyrazine, quinoline; R = H, Cl, Br, F, I, lower alkyl, lower alkoxy, NO2, lower ester, COOH; n = 0, 1, 2; X-Y = CH2S, SCH2, (CH2)2, (CH2)3, (CH2)4, CH2O, S(:O)CH2, CH2S(:O); W = S, O; Q = CH2, CO; R4 = H, OH; R6 = H, C6H5, CH2N(CH3)2, CH2N(CH2CH2)2NCH3; Z = S, O, CH2, (CH2)2, CO, CH(C6H5), CH(4-FC6H4), CHCOOCH2CH3, C(OH)(C6H5), CHOH, CHOCH3, CHOCOCH3; dotted bond = single, double] and pharmaceutically acceptable salts are prepd. as anti-integrase inhibitors useful as treatments for

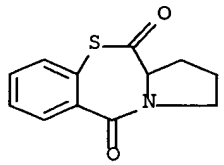
HIV
disease. Thus, the title compd. II was prepd., tested and use as prophylactic treatment against HIV infection.

IT **151433-63-5P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of benzothiazepine as inhibitors of HIV-1 integrase)

RN 151433-63-5 CAPLUS

CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro- (9CI) (CA INDEX NAME)

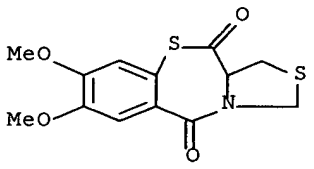


IT **151324-43-5P 151324-45-7P 151324-46-8P**
244610-00-2P 244610-01-3P 244610-04-6P
244610-05-7P 244610-06-8P 244610-08-0P
244610-09-1P 244610-10-4P 244610-13-7P
244610-14-8P 244610-15-9P 244610-16-0P
244610-17-1P 244626-16-2P 244626-17-3P
244626-18-4P 306274-74-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of benzothiazepine as inhibitors of HIV-1 integrase)

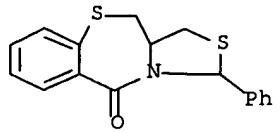
RN 151324-43-5 CAPLUS

CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)

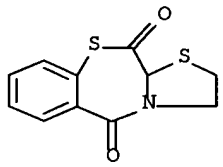


RN 151324-45-7 CAPLUS

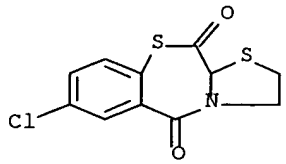
CN 1H,3H,5H-Thiazolo[4,3-c][1,4]benzothiazepin-5-one, 11,11a-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



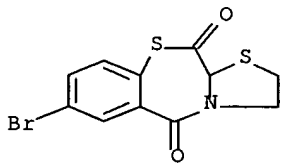
RN 151324-46-8 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)



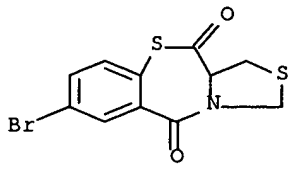
RN 244610-00-2 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-chloro-2,3-dihydro- (9CI) (CA INDEX NAME)



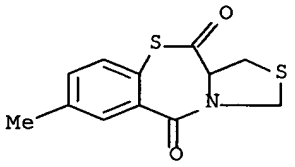
RN 244610-01-3 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 7-bromo-2,3-dihydro- (9CI) (CA INDEX NAME)



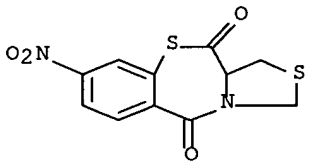
RN 244610-04-6 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-bromo-1,11a-dihydro- (9CI) (CA INDEX NAME)



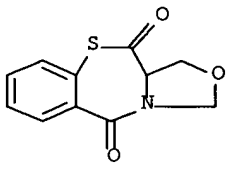
RN 244610-05-7 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methyl- (9CI) (CA INDEX NAME)



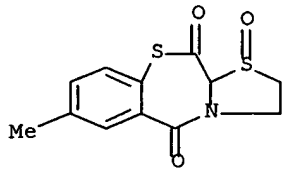
RN 244610-06-8 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-8-nitro- (9CI) (CA INDEX NAME)



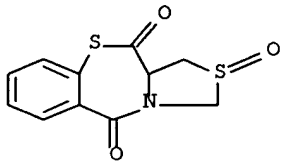
RN 244610-08-0 CAPLUS
CN 3H,5H,11H-Oxazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro- (9CI) (CA INDEX NAME)



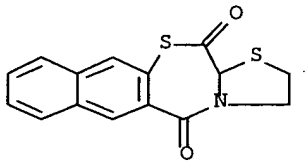
RN 244610-09-1 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl-, 1-oxide (9CI) (CA INDEX NAME)



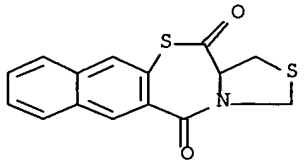
RN 244610-10-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-,
2-oxide (9CI) (CA INDEX NAME)



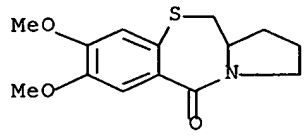
RN 244610-13-7 CAPLUS
CN 5H-Naphtho[2,3-f]thiazolo[2,3-c][1,4]thiazepine-5,13(13aH)-dione,
2,3-dihydro- (9CI) (CA INDEX NAME)



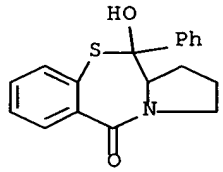
RN 244610-14-8 CAPLUS
CN 3H,5H,13H-Naphtho[2,3-f]thiazolo[4,3-c][1,4]thiazepine-5,13-dione,
1,13a-dihydro- (9CI) (CA INDEX NAME)



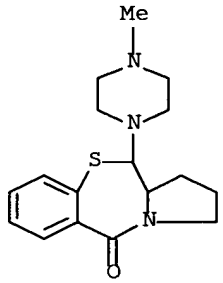
RN 244610-15-9 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-7,8-
dimethoxy- (9CI) (CA INDEX NAME)



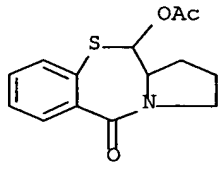
RN 244610-16-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy-11-phenyl- (9CI) (CA INDEX NAME)



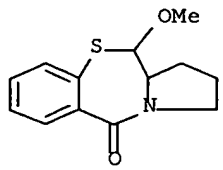
RN 244610-17-1 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



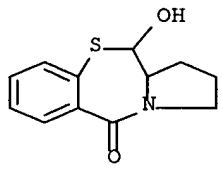
RN 244626-16-2 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-(acetyloxy)-2,3,11,11a-tetrahydro- (9CI) (CA INDEX NAME)



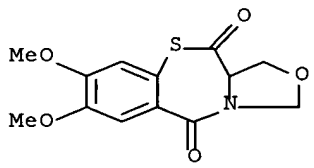
RN 244626-17-3 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-methoxy- (9CI) (CA INDEX NAME)



RN 244626-18-4 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy- (9CI) (CA INDEX NAME)

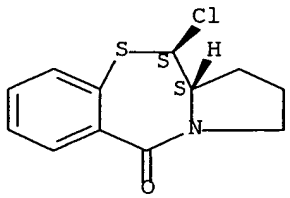


RN 306274-74-8 CAPLUS
CN 3H,5H,11H-Oxazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



IT **149910-60-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzothiazepine as inhibitors of HIV-1 integrase)
RN 149910-60-1 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-chloro-2,3,11,11a-tetrahydro-, (11S,11aS)- (9CI) (CA INDEX NAME)

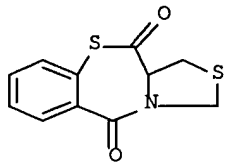
Absolute stereochemistry. Rotation (+).



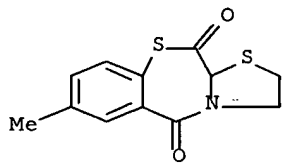
IT **151324-42-4P 244610-02-4P 244610-03-5P**
244610-07-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of benzothiazepine as inhibitors of HIV-1 integrase)

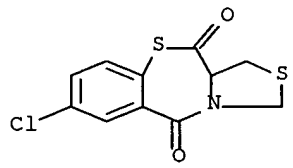
RN 151324-42-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro- (9CI) (CA INDEX NAME)



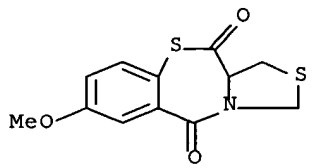
RN 244610-02-4 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl- (9CI) (CA INDEX NAME)



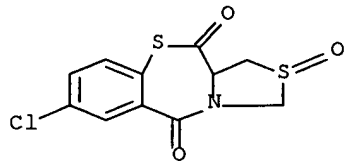
RN 244610-03-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-chloro-1,11a-dihydro- (9CI) (CA INDEX NAME)



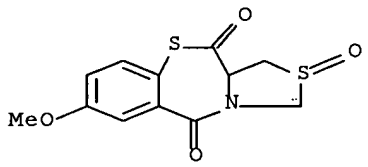
RN 244610-07-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



IT **306274-75-9P 306274-76-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzothiazepine as inhibitors of HIV-1 integrase)
RN 306274-75-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-chloro-1,11a-dihydro-, 2-oxide (9CI) (CA INDEX NAME)

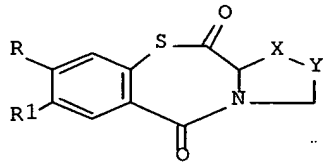


RN 306274-76-0 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy-, 2-oxide (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1999:474380 CAPLUS
DN 131:257538
TI Thiazolothiazepine Inhibitors of HIV-1 Integrase
AU Neamati, Nouri; Turpin, Jim A.; Winslow, Heather E.; Christensen, John L.;
Williamson, Karen; Orr, Ann; Rice, William G.; Pommier, Yves; Garofalo, Antonio; Brizzi, Antonella; Campiani, Giuseppe; Fiorini, Isabella; Nacci, Vito
CS Laboratory of Molecular Pharmacology Division of Basic Sciences, National Cancer Institute, Bethesda, MD, 20892-4255, USA
SO Journal of Medicinal Chemistry (1999), 42(17), 3334-3341
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



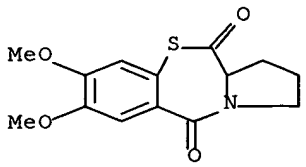
I

AB A series of thiazolothiazepines were prepd. and tested against purified human immunodeficiency virus type-1 integrase (HIV-1 IN) and viral replication. Structure-activity studies reveal that the compds. possessing the pentat. moiety SC(O)CNC(O) with two carbonyl groups are in general more potent against purified IN than those contg. only one carbonyl group. Substitution with electron-donating or -withdrawing groups did not enhance nor abolish potency against purified IN. By contrast, compds. with a naphthalene ring system showed enhanced potency, suggesting that a hydrophobic pocket in the IN active site might accommodate an arom. system rather than a halogen. The position of sulfur in the thiazole ring appears important for potency against IN, as its replacement with an oxygen or carbon abolished activity. Further extension of the thiazole ring diminished potency. I [R, R1 = H, X = S, Y = CH2; RR1 = CH:CHCH:CH; X = S, Y = CH2; X = CH2, Y = S] showed antiviral activity and inhibited IN within similar concns. These compds. inhibited IN when Mn2+ or Mg2+ was used as cofactor. None of these compds. showed detectable activities against HIV-1 reverse transcriptase, protease, virus attachment, or nucleocapsid protein zinc fingers. Therefore, thiazolothiazepines are potentially important lead compds. for

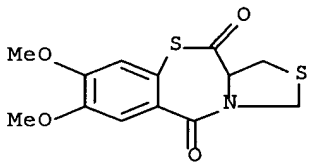
development
as inhibitors of IN and HIV replication.

IT **125262-81-9 151324-43-5 151324-45-7 151324-46-8 151324-47-9 244610-00-2 244610-01-3 244610-15-9 244626-16-2 244626-17-3 244626-18-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of thiazolothiazepines as inhibitors of HIV-1 integrase)

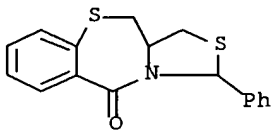
RN 125262-81-9 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



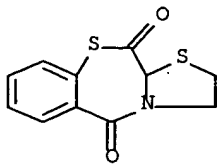
RN 151324-43-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



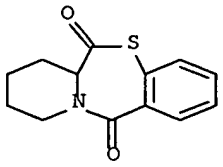
RN 151324-45-7 CAPLUS
CN 1H,3H,5H-Thiazolo[4,3-c][1,4]benzothiazepin-5-one, 11,11a-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



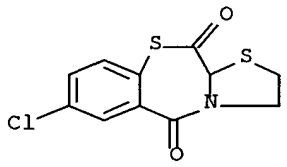
RN 151324-46-8 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)



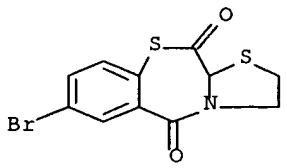
RN 151324-47-9 CAPLUS
CN 12H-Pyrido[2,1-c][1,4]benzothiazepine-6,12(6aH)-dione,
7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)



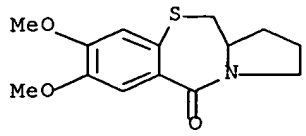
RN 244610-00-2 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione,
7-chloro-2,3-dihydro- (9CI) (CA INDEX NAME)



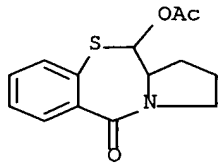
RN 244610-01-3 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione,
7-bromo-2,3-dihydro- (9CI) (CA INDEX NAME)



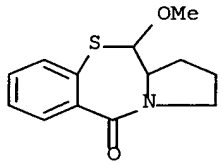
RN 244610-15-9 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-
7,8-
dimethoxy- (9CI) (CA INDEX NAME)



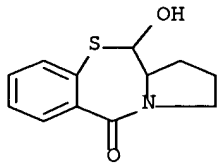
RN 244626-16-2 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-(acetyloxy)-2,3,11,11a-
tetrahydro- (9CI) (CA INDEX NAME)



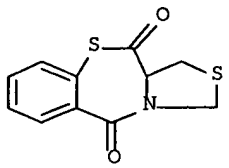
RN 244626-17-3 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-methoxy- (9CI) (CA INDEX NAME)



RN 244626-18-4 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy- (9CI) (CA INDEX NAME)

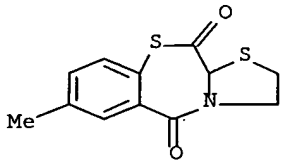


IT **151324-42-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(prepn. of thiazolothiazepines as inhibitors of HIV-1 integrase)
RN 151324-42-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro- (9CI) (CA INDEX NAME)

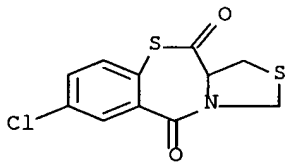


IT **244610-02-4P 244610-03-5P 244610-07-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of thiazolothiazepines as inhibitors of HIV-1 integrase)

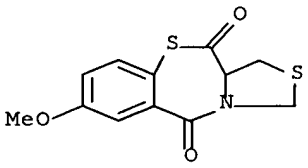
RN 244610-02-4 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-7-methyl- (9CI) (CA INDEX NAME)



RN 244610-03-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-chloro-1,11a-dihydro- (9CI) (CA INDEX NAME)



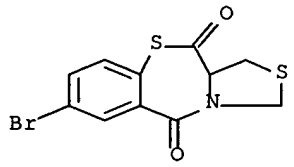
RN 244610-07-9 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methoxy- (9CI) (CA INDEX NAME)



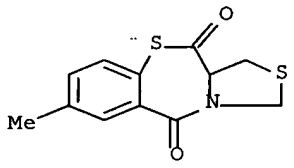
IT **244610-04-6P 244610-05-7P 244610-06-8P**
244610-08-0P 244610-09-1P 244610-10-4P
244610-11-5P 244610-12-6P 244610-13-7P

244610-14-8P 244610-16-0P 244610-17-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of thiazolothiazepines as inhibitors of HIV-1 integrase)

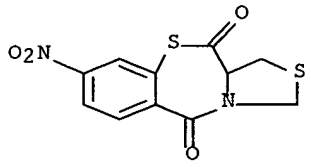
RN 244610-04-6 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 7-bromo-1,11a-dihydro- (9CI) (CA INDEX NAME)



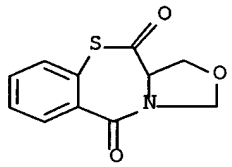
RN 244610-05-7 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7-methyl- (9CI) (CA INDEX NAME)



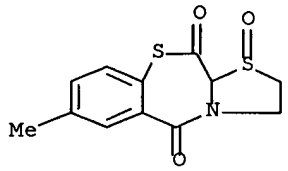
RN 244610-06-8 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-8-nitro- (9CI) (CA INDEX NAME)



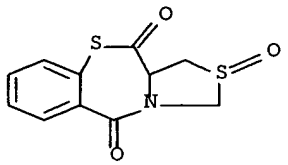
RN 244610-08-0 CAPLUS
CN 3H,5H,11H-Oxazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro- (9CI) (CA INDEX NAME)



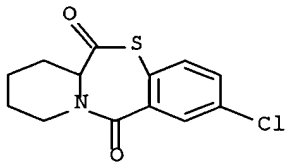
RN 244610-09-1 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione,
2,3-dihydro-7-methyl-, 1-oxide (9CI) (CA INDEX NAME)



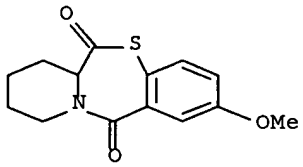
RN 244610-10-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-
,
2-oxide (9CI) (CA INDEX NAME)



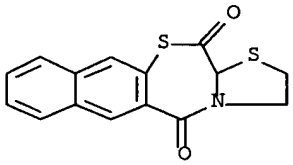
RN 244610-11-5 CAPLUS
CN 12H-Pyrido[2,1-c][1,4]benzothiazepine-6,12(6aH)-dione,
2-chloro-7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)



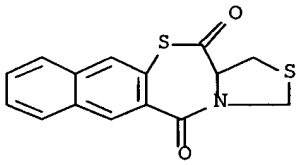
RN 244610-12-6 CAPLUS
CN 12H-Pyrido[2,1-c][1,4]benzothiazepine-6,12(6aH)-dione,
7,8,9,10-tetrahydro-2-methoxy- (9CI) (CA INDEX NAME)



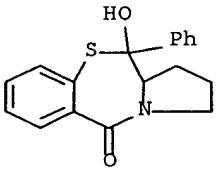
RN 244610-13-7 CAPLUS
CN 5H-Naphtho[2,3-f]thiazolo[2,3-c][1,4]thiazepine-5,13(13aH)-dione, 2,3-dihydro- (9CI) (CA INDEX NAME)



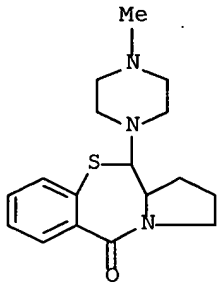
RN 244610-14-8 CAPLUS
CN 3H,5H,13H-Naphtho[2,3-f]thiazolo[4,3-c][1,4]thiazepine-5,13-dione, 1,13a-dihydro- (9CI) (CA INDEX NAME)



RN 244610-16-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy-11-phenyl- (9CI) (CA INDEX NAME)

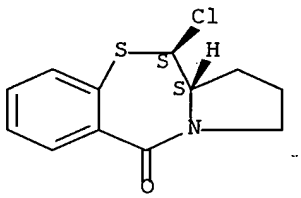


RN 244610-17-1 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-(4-
methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

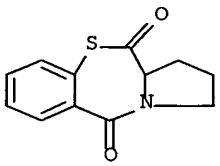


IT **149910-60-1 151433-63-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of thiazolothiazepines as inhibitors of HIV-1 integrase)
RN 149910-60-1 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-chloro-2,3,11,11a-tetrahydro-, (11S,11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

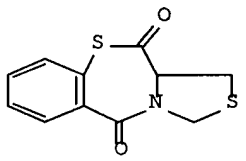


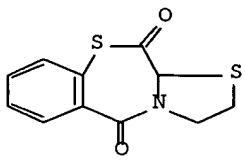
RN 151433-63-5 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-
(9CI) (CA INDEX NAME)

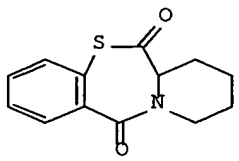


RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1994:8576 CAPLUS
DN 120:8576
TI Thio analogs of anti-tumor antibiotics. II. Synthesis and preliminary in vitro cytotoxicity evaluation of tricyclic [1,4]benzothiazepine derivatives
AU Garofalo, A.; Balconi, G.; Botta, M.; Corelli, F.; D'Incalci, M.; Fabrizi, G.; Fiorini, I.; Lamba, D.; Nacci, V.
CS Dip. Farm. Chim. Tecnol., Univ. Siena, Siena, I-53100, Italy
SO European Journal of Medicinal Chemistry (1993), 28(3), 213-20
CODEN: EJMCA5; ISSN: 0223-5234
DT Journal
LA English
OS CASREACT 120:8576
GI


I

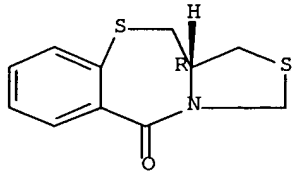

II


III

AB The prepn. of tricyclic [1,4]benzothiazepine derivs. starting from optically active cyclic amino acids and amino alcs. is described. The abs. configurations of the target compds. were assigned by x-ray and 1H-NMR analyses and by mol. modeling studies. The cytotoxic activity of the tricyclic derivs. was tested in vitro by growth inhibition assays using murine L1210 and human lymphoblastic CCRF-CEM leukemias. Compds. I, II, III exhibited marked cytotoxic activity.

IT **151324-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 151324-44-6 CAPLUS
CN 1H,3H,5H-Thiazolo[4,3-c][1,4]benzothiazepin-5-one, 11,11a-dihydro-, (R)- (9CI) (CA INDEX NAME)

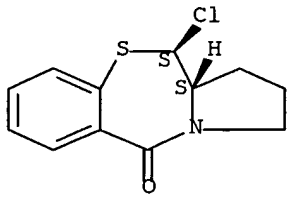
Absolute stereochemistry.



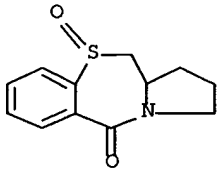
IT **149910-60-1P 151324-60-6P 151433-64-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for benzothiazepine anthramycin analog (neoplasm inhibitor))
RN 149910-60-1 CAPLUS

CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-chloro-2,3,11,11a-tetrahydro-, (11S,11aS)- (9CI) (CA INDEX NAME)

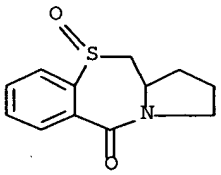
Absolute stereochemistry. Rotation (+).



RN 151324-60-6 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-, 10-oxide, (10S-cis)- (9CI) (CA INDEX NAME)

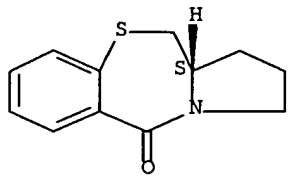


RN 151433-64-6 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-, 10-oxide, (10R-trans)- (9CI) (CA INDEX NAME)

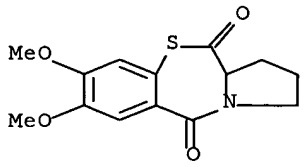


IT **121451-33-0P 125262-81-9P 125262-82-0P**
125262-88-6P 149910-58-7P 149910-59-8P
149910-61-2P 151324-42-4P 151324-43-5P
151324-45-7P 151324-46-8P 151324-47-9P
151433-63-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as neoplasm inhibitor)
RN 121451-33-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-, (11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

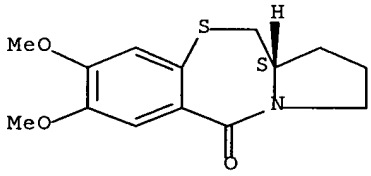


RN 125262-81-9 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-
7,8-dimethoxy- (9CI) (CA INDEX NAME)



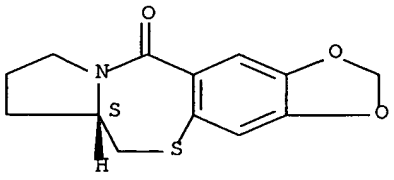
RN 125262-82-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-7,8-
dimethoxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 125262-88-6 CAPLUS
CN 6H,11H-1,3-Dioxolo[4,5-h]pyrrolo[2,1-c][1,4]benzothiazepin-11-one,
6a,7,8,9-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

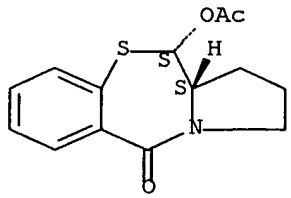
Absolute stereochemistry.



RN 149910-58-7 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-(acetyloxy)-

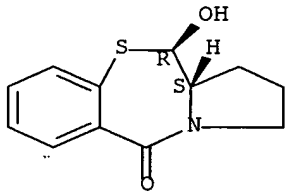
2,3,11,11a-
tetrahydro-, (11S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



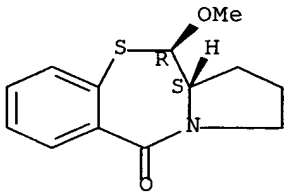
RN 149910-59-8 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy-, (11R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

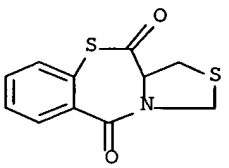


RN 149910-61-2 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-methoxy-, (11R-cis)- (9CI) (CA INDEX NAME)

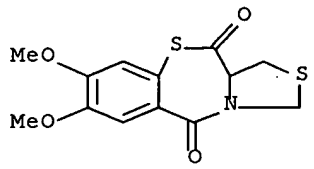
Absolute stereochemistry.



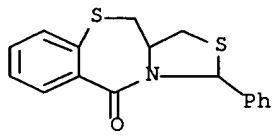
RN 151324-42-4 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro- (9CI) (CA INDEX NAME)



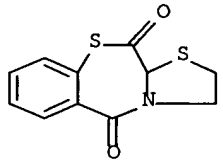
RN 151324-43-5 CAPLUS
CN 3H,5H,11H-Thiazolo[4,3-c][1,4]benzothiazepine-5,11-dione, 1,11a-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)



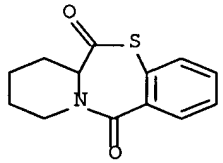
RN 151324-45-7 CAPLUS
CN 1H,3H,5H-Thiazolo[4,3-c][1,4]benzothiazepin-5-one, 11,11a-dihydro-3-phenyl-(9CI) (CA INDEX NAME)



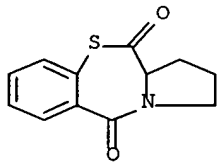
RN 151324-46-8 CAPLUS
CN 5H-Thiazolo[2,3-c][1,4]benzothiazepine-5,11(11aH)-dione, 2,3-dihydro-(9CI) (CA INDEX NAME)



RN 151324-47-9 CAPLUS
CN 12H-Pyrido[2,1-c][1,4]benzothiazepine-6,12(6aH)-dione, 7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)

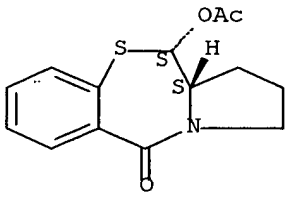


RN 151433-63-5 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-(9CI) (CA INDEX NAME)



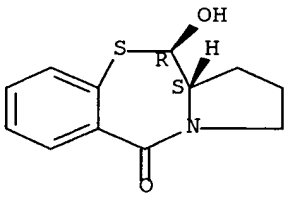
L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1993:539145 CAPLUS
DN 119:139145
TI Benzothiazine and benzothiazepine derivatives: Synthesis and preliminary biological evaluation
AU Garofalo, Antonio; Campiani, Giuseppe; Fiorini, Isabella; Nacci, Vito
CS Dip. Farm. Chim. Technol., Univ. Siena, Siena, 53100, Italy
SO Farmaco (1993), 48(2), 275-83
CODEN: FRMCE8; ISSN: 0014-827X
DT Journal; General Review
LA English
AB A review of the author's recent work on the prepn. of tricyclic benzothiazines and benzothiazepines via intramol. cyclization reactions and their functionalization to biol. active compds.
IT **149910-58-7P 149910-59-8P 149910-60-1P**
149910-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and functionalization of, biol. compds. from)
RN 149910-58-7 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-(acetyloxy)-2,3,11,11a-tetrahydro-, (11S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



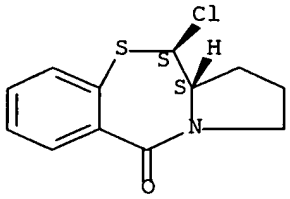
RN 149910-59-8 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-hydroxy-, (11R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



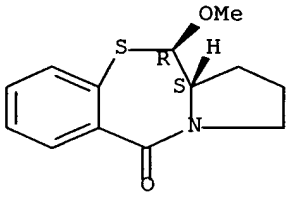
RN 149910-60-1 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 11-chloro-2,3,11,11a-tetrahydro-, (11S,11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

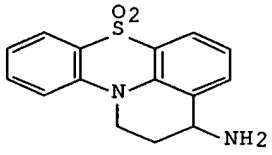


RN 149910-61-2 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-11-methoxy-, (11R-cis)- (9CI) (CA INDEX NAME)

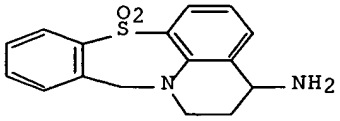
Absolute stereochemistry.



L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1991:656136 CAPLUS
DN 115:256136
TI Synthesis of 3-amino-2,3-dihydro-1H-pyrido[3,2,1-kl]phenothiazine 5,5-dioxide and of 3-amino-1,2-dihydro-3H-dibenzo[c,jk]pyrido[2,1-c]-1,4-thiazepine 7,7-dioxide
AU Catsoulacos, P.; Pelecanou, M.; Camoutsis, C.
CS Sch. Health Sci., Univ. Patras, Patras, 26500, Greece
SO Journal of Heterocyclic Chemistry (1991), 28(5), 1437-40
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
GI



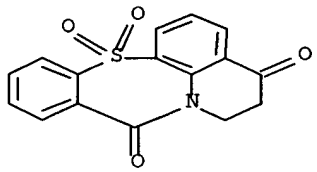
I



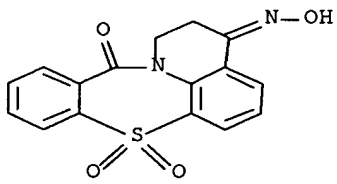
II

AB 3-Aminopyrido[3,2,1-kl]phenothiazine 5,5-dioxide I and aminodibenzo[c,jk]pyrido[2,1-c]thiazepine 7,7-dioxide II were synthesized from the corresponding 3-oxime acetates by redn. with the borane-tetrahydrofuran complex. Redn. was not successful in the case of 2,3-dihydro-1H-pyrido[3,2,1-kl]phenothiazine-3-oxime acetate.

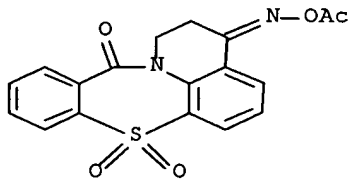
IT **43168-21-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oximation of)
RN 43168-21-4 CAPLUS
CN 3H,12H-Quino[8,1-bc][1,4]benzothiazepine-3,12-dione, 1,2-dihydro-, 7,7-dioxide (9CI) (CA INDEX NAME)



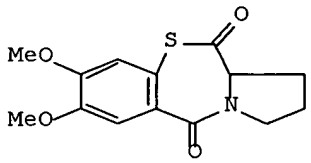
IT **137279-78-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)(prepn. and acetylation of)
RN 137279-78-8 CAPLUS
CN 1H,12H-Quino[8,1-bc][1,4]benzothiazepine-3,12(2H)-dione, 3-oxime, 7,7-dioxide (9CI) (CA INDEX NAME)



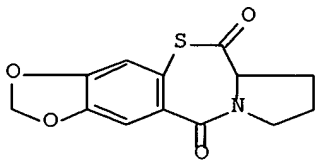
IT **137279-79-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)
RN 137279-79-9 CAPLUS
CN 1H,12H-Quino[8,1-bc][1,4]benzothiazepine-3,12(2H)-dione, 3-(O-acetyloxime), 7,7-dioxide (9CI) (CA INDEX NAME)



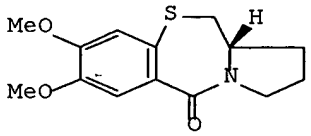
L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1990:98498 CAPLUS
DN 112:98498
TI Thioanalogs of antitumor antibiotics. I. Synthesis of 7,8-disubstituted
5,11-dioxo-1,2,3,11a-tetrahydro-5H,11H- and 5-oxo-2,3,11,11a-tetrahydro-1H,5H-pyrrolo[2,1-c][1,4]benzothiazepine
AU Nacci, V.; Garofalo, A.; Anzini, M.
CS Dip. Farm. Chim. Tecnol., Univ. Siena, Siena, Italy
SO Farmaco (1989), 44(4), 423-33
CODEN: FRMCE8; ISSN: 0014-827X
DT Journal
LA English
OS CASREACT 112:98498
GI



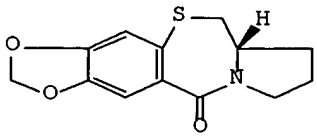
I



II

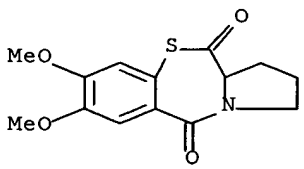


III



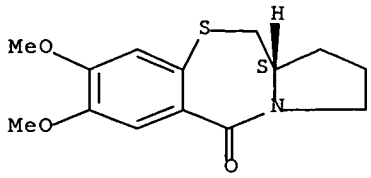
IV

AB The synthesis of 7,8-dimethoxy-5,11-dioxo-1,2,3,11a-tetrahydro-5H,11H-pyrrolo[2,1-c][1,4]benzothiazepine (I), 6,11-dioxo-6a,7,8,9-tetrahydro-6H,11H-[1,3]dioxolo[4,5-h]pyrrolo[2,1-c][1,4]benzothiazepine (II), (11aS)-7,8-dimethoxy-5-oxo-2,3,11,11a-tetrahydro-1H,5H-pyrrolo[2,1-c][1,4]benzothiazepine (III) and (6aS)-11-oxo-6a,7,8,9-tetrahydro-6H,11H-
[1,3]dioxolo[4,5-h]pyrrolo[2,1-c][1,4]benzothiazepine (IV) are reported.
IT **125262-81-9P 125262-82-0P 125262-87-5P**
125262-88-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 125262-81-9 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-
7,8-dimethoxy- (9CI) (CA INDEX NAME)

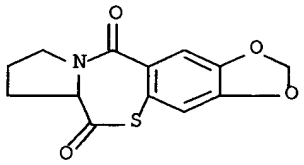


RN 125262-82-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-7,8-
dimethoxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

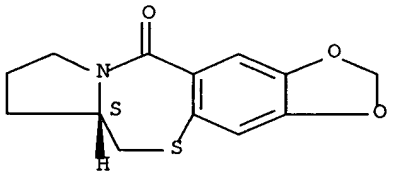


RN 125262-87-5 CAPLUS
CN 6H,11H-1,3-Dioxolo[4,5-h]pyrrolo[2,1-c][1,4]benzothiazepine-6,11-dione, 6a,7,8,9-tetrahydro- (9CI) (CA INDEX NAME)

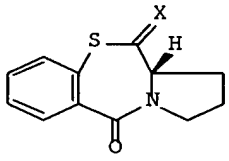


RN 125262-88-6 CAPLUS
CN 6H,11H-1,3-Dioxolo[4,5-h]pyrrolo[2,1-c][1,4]benzothiazepin-11-one, 6a,7,8,9-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1989:439326 CAPLUS
DN 111:39326
TI Polycondensed heterocycles. III. Synthesis of 5,11-dioxo-1,2,3,11a-tetrahydro-5H,11H- and 5-oxo-2,3,11,11a-tetrahydro-1H,5H-pyrrolo[2,1-c][1,4]benzothiazepine
AU Nacci, V.; Garofalo, A.; Anzini, M.; Campiani, G.
CS Dip. Farm. Chim. Tecnol., Univ. Siena, Siena, 53100, Italy
SO Journal of Heterocyclic Chemistry (1988), 25(3), 1007-13
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 111:39326
GI

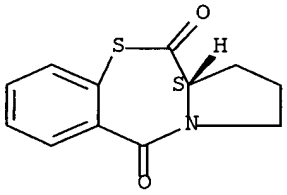


I

AB The title compds. I (X = O, H2) were prepd. in several steps by cyclocondensation of L-proline or (S)-prolinol derivs. resp., with 2-(methylthio)benzoic acid derivs. I have structures similar to several benzodizaepine antitumor antibiotics.

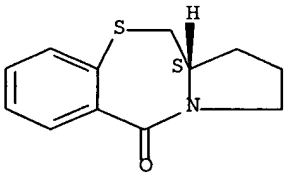
IT **104207-34-3P 121451-33-0P**
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
RN 104207-34-3 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 121451-33-0 CAPLUS
CN 1H,5H-Pyrrolo[2,1-c][1,4]benzothiazepin-5-one, 2,3,11,11a-tetrahydro-, (11aS)- (9CI) (CA INDEX NAME)

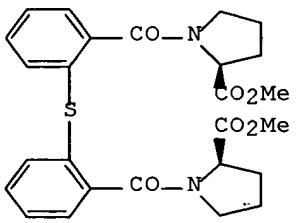
Absolute stereochemistry. Rotation (+).



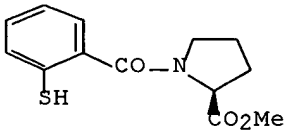
L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1986:533532 CAPLUS
DN 105:133532
TI Aromatic N-substituted amide derivatives
IN Morisawa, Yasuhiro; Nishi, Takehide; Tsujita, Yoshio
PA Sankyo Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 61068457	A2	19860408	JP 1984-190477	19840913
PRAI JP 1984-190477		19840913		

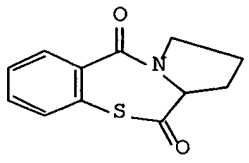
OS CASREACT 105:133532
GI



II



III



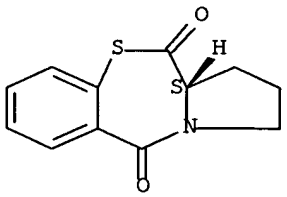
IV

AB o-RC6H4CONR1CR2R3CO2R4 [I; OH, SH, acylthio, CO2H, alkoxycarbonyl, RR4 may form thiolactone ring; R1 = (un)substituted alkyl, cycloalkyl, arom. condensed cycloalkyl, aryl, aralkyl, heterocyclic ring, heterocyclic alkyl; R1R2 may form (arom. condensed) 5-6-membered ring; R2, R3 = H, alkyl; R4 = H, protective group] and pharmacol. permissible salts of I, useful as antihypertensives via inhibiting effects on angiotensin converting enzyme, were prepd. Thus, refluxing bis(2-carboxyphenyl) disulfide with L-proline Me ester HCl salt in anhyd. THF gave 67% II, which was reduced using Ph3P in dioxane to give 74% III. Then III was deprotected and treated with DCC n the presence of 4-(dimethylamino)pyridine to give 94% title compd. IV, which showed IC50 against angiotensin converting enzyme at 8.5 .times. 10-6 mol/L in vitro.

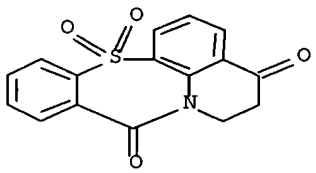
IT **104207-34-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as antihypertensive)

RN 104207-34-3 CAPLUS
CN 5H,11H-Pyrrolo[2,1-c][1,4]benzothiazepine-5,11-dione, 1,2,3,11a-tetrahydro-
, (S)- (9CI) (CA INDEX NAME)

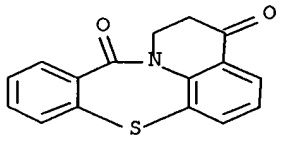
Absolute stereochemistry.



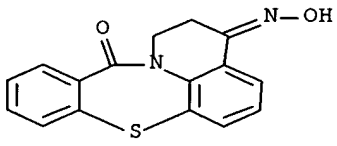
L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1973:515543 CAPLUS
DN 79:115543
TI Synthesis of dibenzo[b,f]-1,4-thiazepin-10-one 5,5-dioxide derivatives
AU Catsoulacos, P.
CS Lab. Chem. Pharm., Univ. Athens, Athens, Greece
SO Bulletin de la Societe Chimique de France (1973), (6)(Pt. 2), 2136-7
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
GI For diagram(s), see printed CA Issue.
AB The dibenzothiazepinone dioxide I (R = H) was prepd. by Beckmann rearrangement of 10-(hydroxyimino)thioxanthene 5,5-dioxide. Treating I (R = H) with CH2:CHCN gave I (R = CH2CH2CN), which was hydrolyzed to I (R = CH2CH2CO2Me, CH2CH2CO2H), both of which were cyclized with POCl3 to the dibenzopyridothiazepinedione dioxide II. Reaction of II with NaN3-H3PO4 gave 1,2,3,4-tetrahydrodibenzo[c,kl][1,4]diazepino[2,1-c][1,4]thiazepine-3,13-dione 8,8-dioxide (III).
IT **43168-21-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 43168-21-4 CAPLUS
CN 3H,12H-Quino[8,1-bc][1,4]benzothiazepine-3,12-dione, 1,2-dihydro-, 7,7-dioxide (9CI) (CA INDEX NAME)



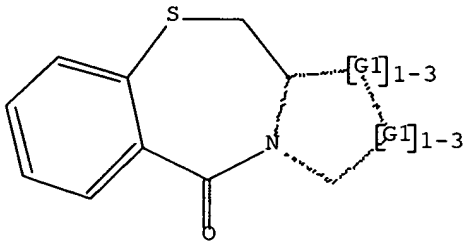
L4 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS
AN 1972:34228 CAPLUS
DN 76:34228
TI Syntheses of heterocyclic compounds involving sulfur. III. Synthesis of
4-methyl-1,2,3,4-tetrahydrodibenzo[c,Kl]-1,4-diazepino[2,1-c]-1,4-thiazepine
AU Shirai, Hideaki; Hayazaki, Takanori; Maki, Akemichi
CS Fac. Pharm. Sci., Nagoya City Univ., Nagoya, Japan
SO Yakugaku Zasshi (1971), 91(11), 1228-32
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Japanese
AB Dehydrative cyclization of 3-[11-oxodibenzo[b,f]-1,4-thiazepin-10-yl]propionic acid, obtained by hydrolysis of 10-(.beta.-cyanoethyl)dibenzo[b,f]-1,4-thiazepin-11-one with HCl, with P2O5 afforded
1,2-dihydro-3H-dibenzo[c,jk]pyrido[2,1-c]-1,4-thiazepine-3,12-dione (I). The Schmidt reaction of I gave 1,2,3,4-tetrahydrodibenzo[c,kl]-1,4-diazepino[2,1-c]-1,4-thiazepine-3,13-dione (II) and the Me compd. of II was reduced with LiAlH4 to 4-methyl-1,2,3,4-tetrahydrodibenzo[c,kl]-1,4-diazepino-[2,1-c]-1,4-thiazepine (I).
IT **34752-73-3P 34752-78-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 34752-73-3 CAPLUS
CN 3H,12H-Quino[8,1-bc][1,4]benzothiazepine-3,12-dione, 1,2-dihydro- (9CI) (CA INDEX NAME)



RN 34752-78-8 CAPLUS
CN 3H,12H-Quino[8,1-bc][1,4]benzothiazepine-3,12-dione, 1,2-dihydro-, 3-oxime
(9CI) (CA INDEX NAME)



=> d l1; d his; log y
L1 HAS NO ANSWERS
L1 STR



G1 C,O,S

Structure attributes must be viewed using STN Express query preparation.

(FILE 'REGISTRY' ENTERED AT 17:52:28 ON 08 MAY 2003)
DEL HIS
L1 STRUCTURE UPLOADED
L2 3 S L1
L3 48 S L1 FUL

FILE 'CAPLUS' ENTERED AT 17:53:48 ON 08 MAY 2003
L4 15 S L3

FILE 'BEILSTEIN' ENTERED AT 17:54:32 ON 08 MAY 2003
L5 2 S L1
L6 49 S L1 FUL
L7 42 S L6 NOT L3
L8 42 S L6 NOT L4 duplicate of CAPLUS

FILE 'MARPAT' ENTERED AT 17:56:08 ON 08 MAY 2003

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.40	1475.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-9.77

STN INTERNATIONAL LOGOFF AT 17:56:22 ON 08 MAY 2003